

# Using Concurrent Function Evaluations to Identify Local Minima of a Derivative-free Optimization Problem

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August 12, 2015



#### Motivation

▶ We want to identify distinct, "high-quality", local minimizers of

minimize 
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 $x \in \mathbb{R}^n$ 

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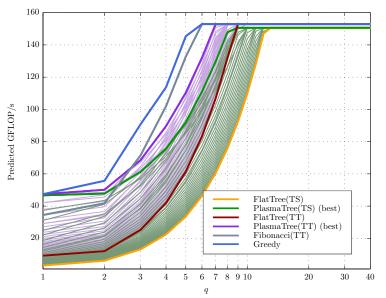
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- High-quality can be measured by more than the objective.
- Derivatives of f may or may not be available.
- ► The simulation *f* is likely using parallel resources, but it does not utilize the entire machine.

## Why concurrency? Tiled QR example



[Bouwmeester, et al., Tiled QR Factorization Algorithms, 2011]

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The theory can be more than merely checking that a method generates iterates which are dense in the domain.

Given some local optimization routine  $\mathcal{L}$ :

#### **Algorithm 1:** General Multistart

**for** k = 1, 2, ... **do** 

Evaluate f at N points drawn from  $\mathcal{D}$ 



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- If resources are limited, how should points from each run receive priority?
- Ideally, only one run is started for each minima.
- **Exploring by sampling.** Refining with  $\mathcal{L}$ .

Given some local optimization routine  $\mathcal{L}$ :

#### Algorithm 2: MLSL

for k = 1, 2, ... do

Sample f at N random points drawn uniformly from  $\mathcal{D}$ Start  $\mathcal{L}$  at all sample points x:

- that has yet to start a run
- ▶  $\nexists x_i : ||x x_i|| \le r_k$  and  $f(x_i) < f(x)$

[Rinnooy Kan and Timmer, Mathematical Programming, 39(1):57-78, 1987]



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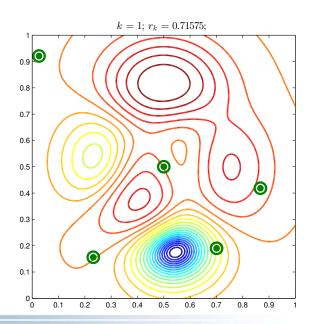
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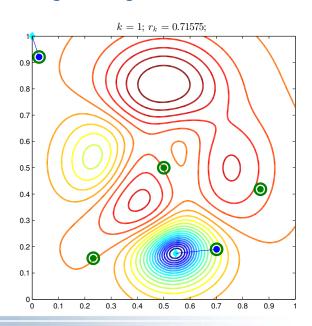
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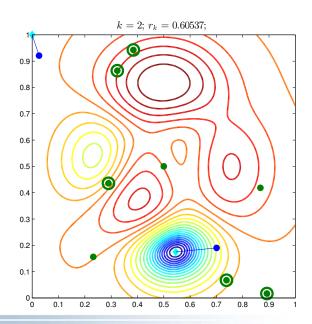
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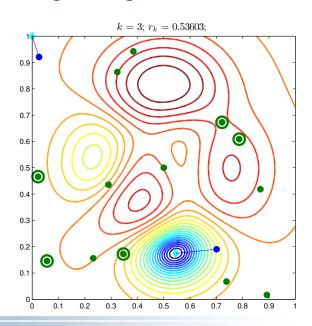
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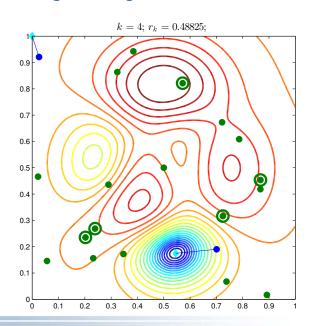
- ▶ Doesn't naturally translate when evaluations of *f* are limited
- ightharpoonup Ignores some points when deciding where to start  ${\cal L}$

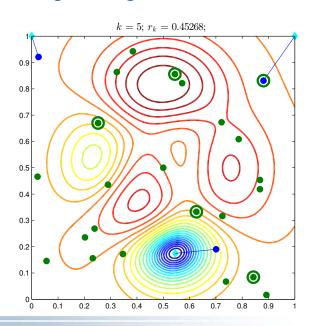


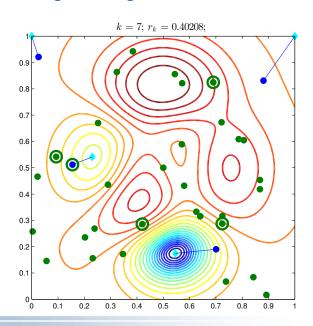


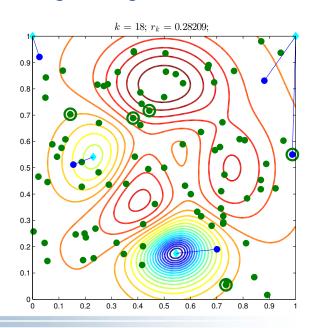


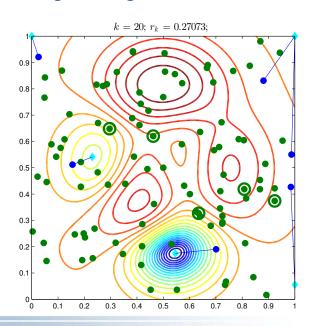


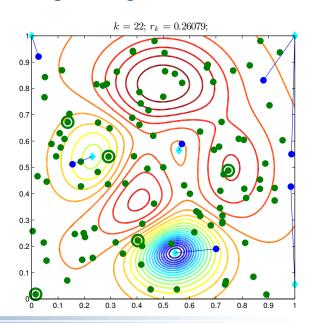












- ▶  $f \in C^2$ , with local minima in the interior of  $\mathcal{D}$ , and the distance between these minima is bounded away from zero.
- $ightharpoonup \mathcal{L}$  is strictly descent and converges to a minimum (not a stationary point).

$$r_k = \frac{1}{\sqrt{\pi}} \sqrt[n]{\Gamma\left(1 + \frac{n}{2}\right) \operatorname{vol}(\mathcal{D})} \frac{\sigma \log kN}{kN}$$
 (1)

#### Theorem

If  $r_k \to 0$ , all local minima will be found almost surely.

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#### Theorem

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If  $r_k$  is defined by (1) with  $\sigma > 4$ , even if the sampling continues forever, the total number of local searches started is finite almost surely.

$$\hat{x} \in \mathcal{S}_k$$

- (S2)  $\nexists x \in S_k$  with  $[\|\hat{x} x\| \le r_k \text{ and } f(x) < f(\hat{x})]$
- (S3)  $\hat{x}$  has not started a local optimization run
- (S4)  $\hat{x}$  is at least  $\mu$  from  $\partial \mathcal{D}$  and  $\nu$  from known local minima



#### MLSL: (S2)-(S4)

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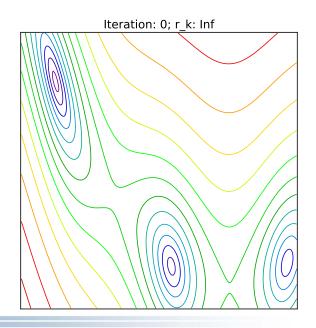
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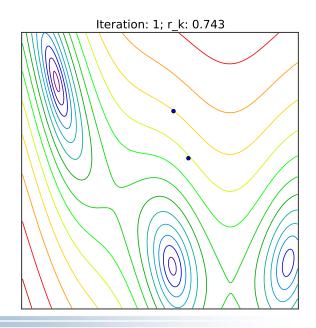
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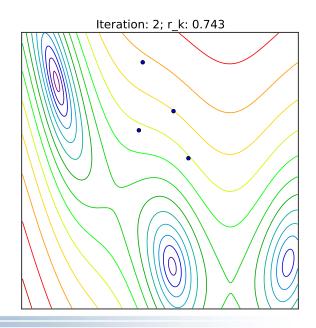
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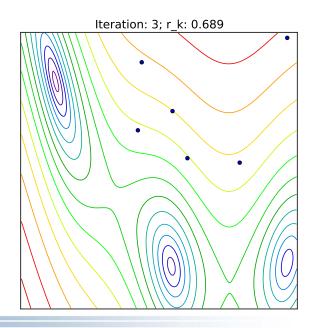
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- (L6)  $\exists r_k$ -descent path in  $\mathcal{H}_k$  from some  $x \in \mathcal{S}_k$  satisfying (S2-S4) to  $\hat{x}$

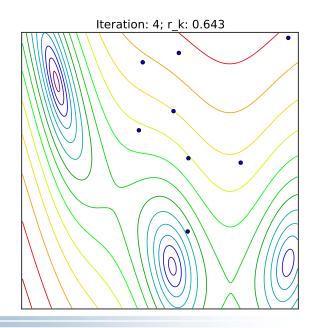


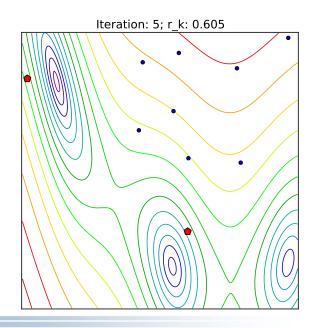


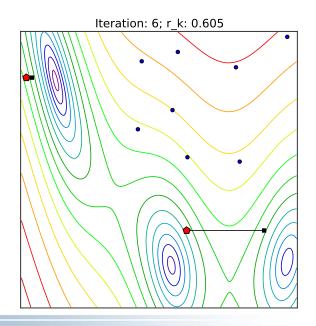


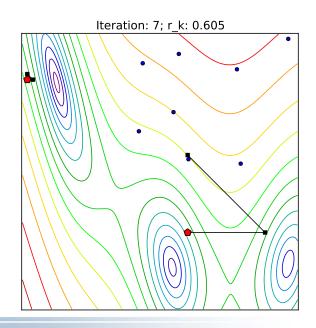


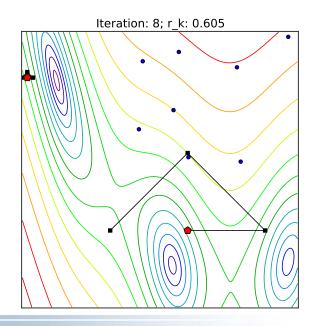


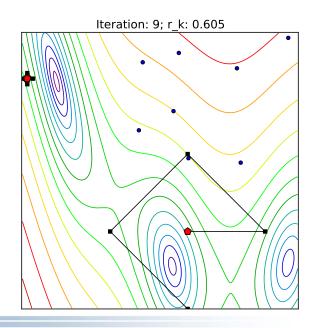


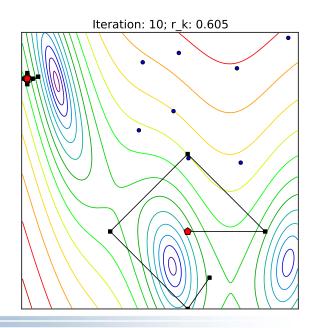


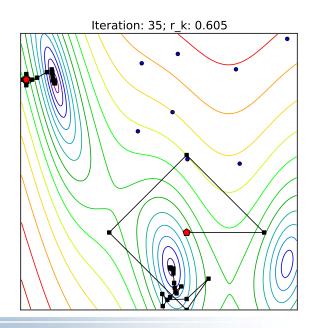


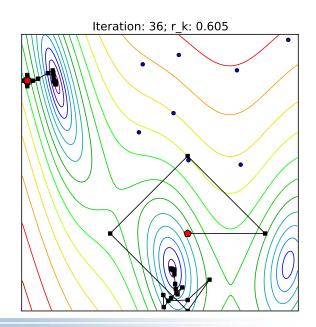


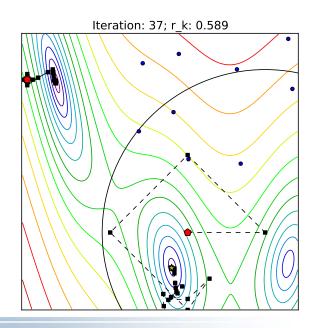


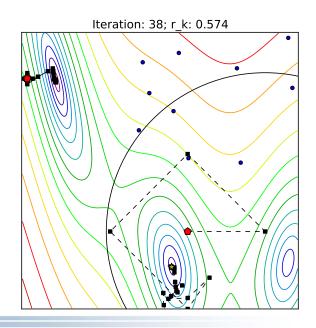


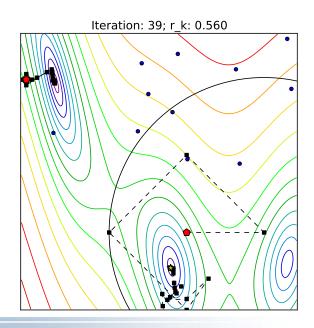


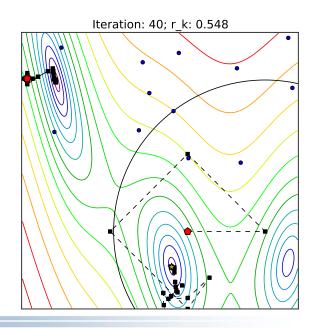


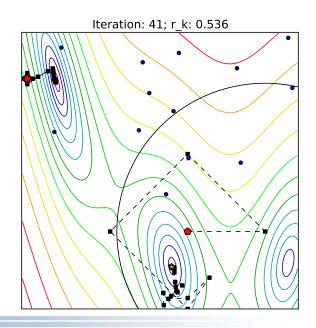


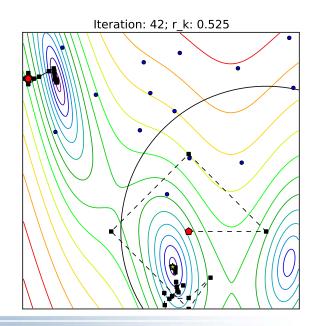


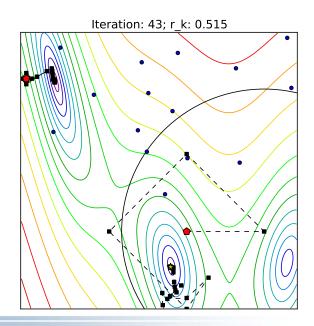


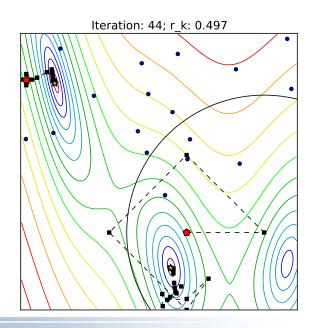


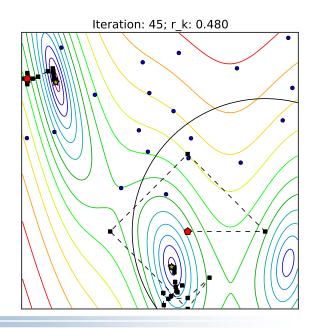


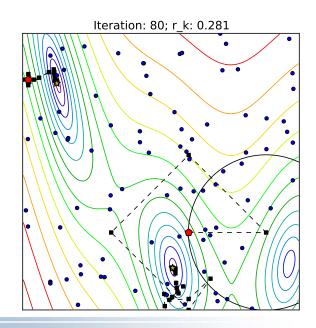


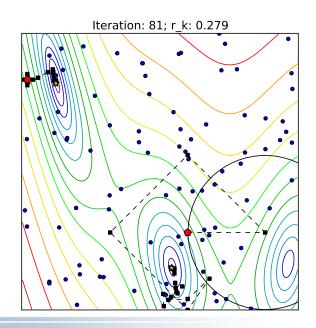


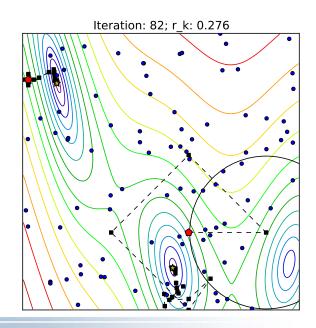


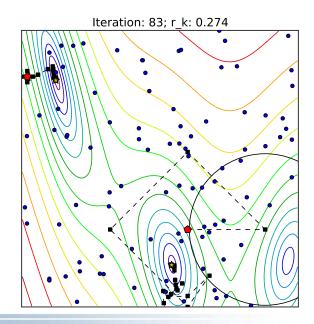


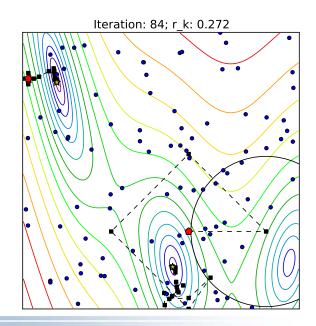


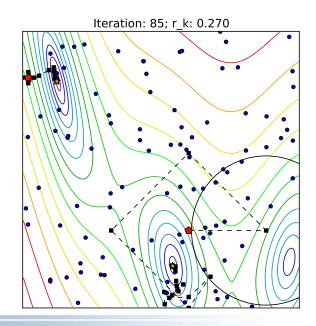


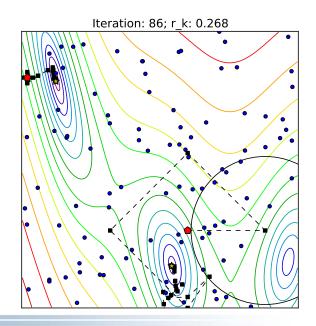


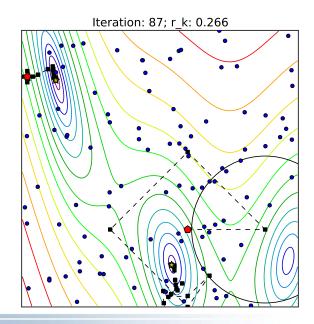


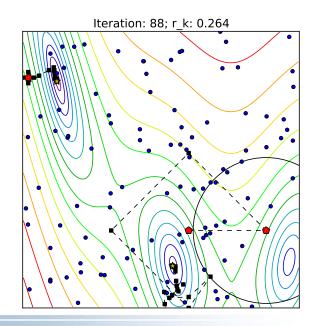


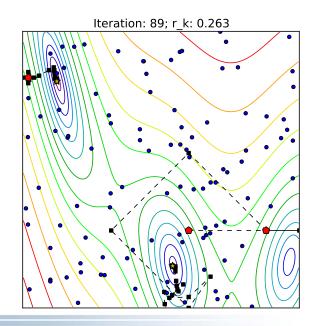


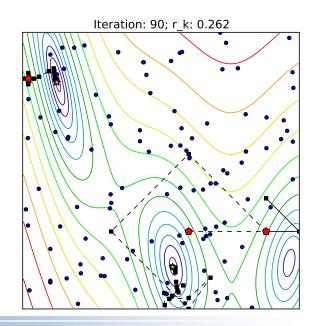


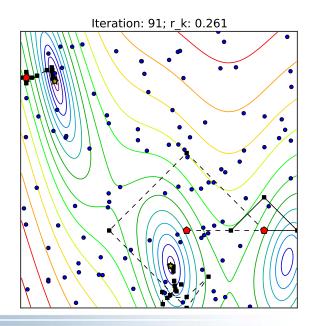


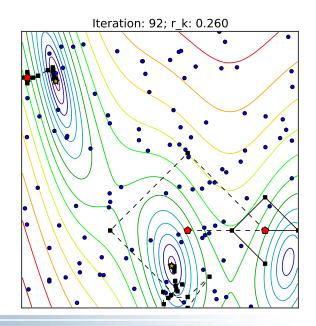


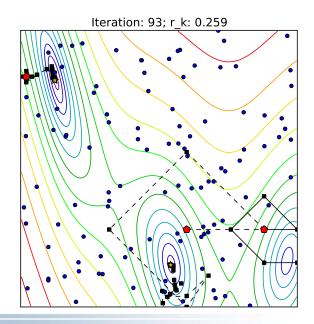


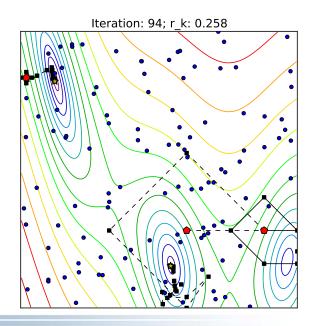


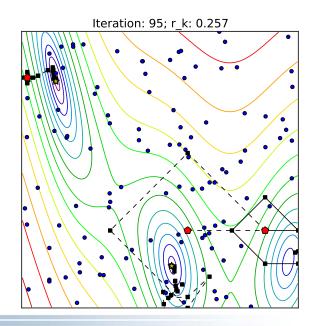


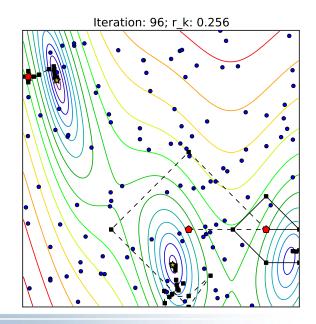


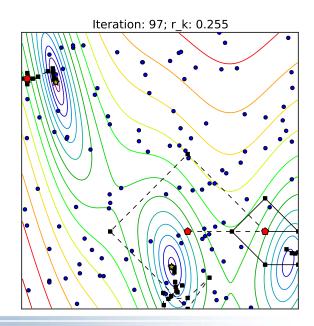


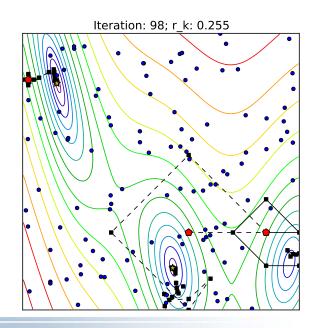


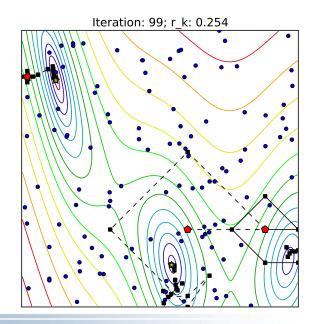












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#### Possibly beneficial:

- Can return multiple points of interest
- Reports solution quality/confidence at every iteration
- Can avoid certain regions in the domain
- Uses a history of past evaluations of f
- Uses additional points mid-run

#### **AAMLM**

#### Algorithm 3: AAMLM

```
Give each worker a point to evaluate
for k = 1, 2, ... do
    Receive from (longest waiting) worker w that has evaluated f
   Update \mathcal{H}_{k} and r_{k}
   if point evaluated by w is from an active run then
       if Run is complete then
           Update X_{\nu}^*, and mark points inactive
       else
           Add the next point in its localopt run (not in \mathcal{H}_k) to Q_L
       Start run(s) at all point(s) satisfying (S1)-(S4), (L1)-(L6)
       Add the subsequent point (not in \mathcal{H}_k) from each run to Q_L
    Merge runs in Q_I with candidate minima within 2\nu of each other
    Give w a point at which to evaluate f, either from Q_I or \mathcal{R}
```

#### **BAMLM**

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#### Theorem

Each  $x^* \in X^*$  will almost surely be either identified in a finite number of evaluations or have a single local optimization run that is converging asymptotically to it.

# Measuring Performance

```
GLODS Global & local optimization using direct search [Custódio, Madeira
      (JOGO, 2014)]
    Direct Serial DIRECT [D. Finkel's MATLAB code]
pVTDirect Parallel DIRECT [He, Watson, Sosonkina (TOMS, 2009)]
  Random Uniform sampling over domain (as a baseline)
  BAMLM
        Concurrency: 4
        Local optimization method
             ▶ ORBIT [Wild, Regis, & Shoemaker (SIAM JOSC, 2008)]
             ► BOBYQA [Powell, 2009]
        ▶ Initial sample size: 10n
```

Each method evaluates Direct's 2n + 1 initial points.

# Measuring Performance

Let  $X^*$  be the set of all local minima of f.

Let  $f_{(i)}^*$  be the *i*th smallest value  $\{f(x^*)|x^*\in X^*\}$ . Let  $x_{(i)}^*$  be the element of  $X^*$  corresponding to the value  $f_{(i)}^*$ .

The global minimum has been found at a level  $\tau > 0$  at batch k if an algorithm it has found a point  $\hat{x}$  satisfying:

$$f(\hat{x}) - f_{(1)}^* \le (1 - \tau) \left( f(x_0) - f_{(1)}^* \right),$$

where  $x_0$  is the starting point for problem p.



# Measuring Performance

Let  $X^*$  be the set of all local minima of f.

Let  $f_{(i)}^*$  be the *i*th smallest value  $\{f(x^*)|x^* \in X^*\}$ . Let  $x_{(i)}^*$  be the element of  $X^*$  corresponding to the value  $f_{(i)}^*$ .

The j best local minima have been found at a level  $\tau > 0$  at batch k if:

$$\left|\left\{x_{(1)}^*, \dots, x_{(\underline{j}-1)}^*\right\} \bigcap \left\{x_{(i)}^* : \exists x \in \mathcal{H}_k \text{ with } \left\|x - x_{(i)}^*\right\| \leq r_n(\tau)\right\}\right| = \underline{j} - 1$$

$$\left|\left\{x_{(\underline{j})}^*, \dots, x_{(\overline{j})}^*\right\} \bigcap \left\{x_{(i)}^* : \exists x \in \mathcal{H}_k \text{ with } \left\|x - x_{(i)}^*\right\| \leq r_n(\tau)\right\}\right| \geq \underline{j} - \underline{j} + 1,$$

where j and  $\bar{j}$  are the smallest and largest integers such that

$$f_{(j)}^* = f_{(j)}^* = f_{(j)}^*$$
 and where  $r_n(\tau) = \sqrt[n]{rac{ au \operatorname{vol}(\mathcal{D})\Gamma(rac{n}{2}+1)}{\pi^{n/2}}}$ .

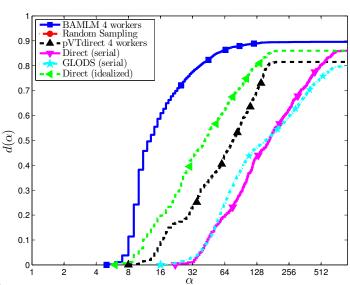


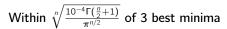
#### Problems considered

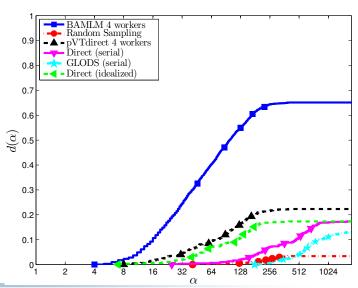
GKLS problem generator [Gaviano et al., "Algorithm 829" (TOMS, 2003)]

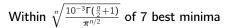
- ▶ 600 synthetic problems with known local minima
- ▶ n = 2.....7
- ▶ 10 local minima in the unit cube with a unique global minimum
- ▶ 100 problems for each dimension
- ▶ 5 replications (different seeds) for each problem
- ▶ 5000 evaluations

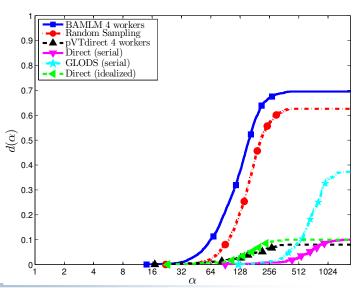
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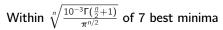


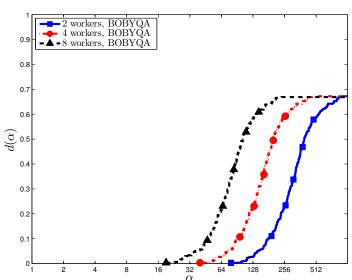


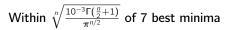


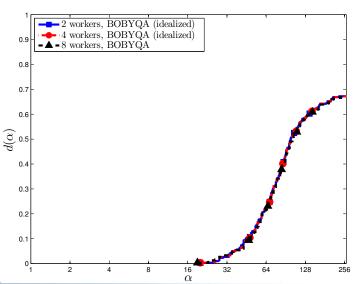


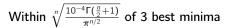


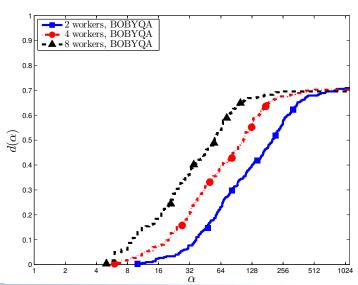


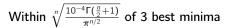


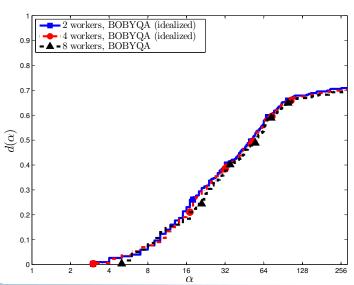


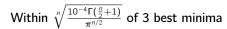


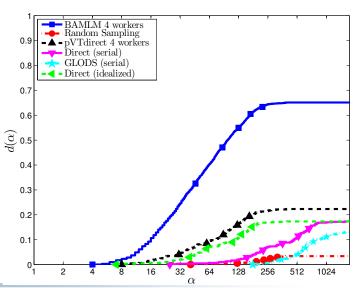




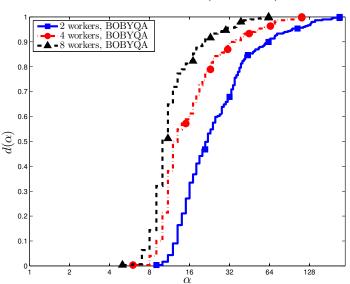




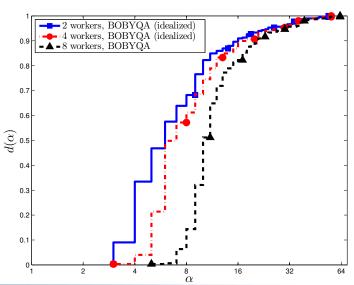




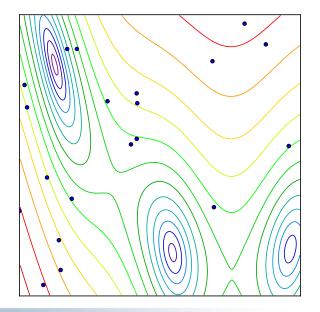
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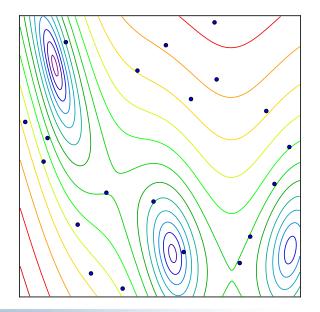


# **Uniform sampling**



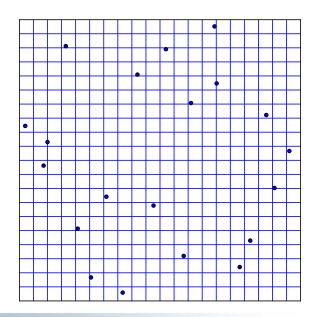


# Latin hypercube sampling





# Latin hypercube sampling





#### **BAMLM** with LHS

Critical distance for uniform sampling:

$$r_k = \pi^{-1/2} \left( \Gamma(1 + \frac{n}{2}) \operatorname{vol}(\mathcal{D}) \frac{\sigma \log kN}{kN} \right)^{1/n}$$

Critical distance for Latin hypercube sampling:

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#### Theorem

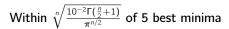
If  $r_k$  is defined by (2) with  $\sigma > 4$ , even if the sampling continues forever, the total number of local runs started by BAMLM (or AAMLM) is finite almost surely.

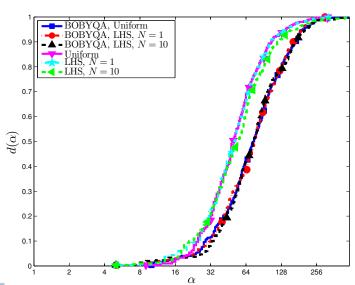


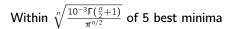
# Does LHS help?

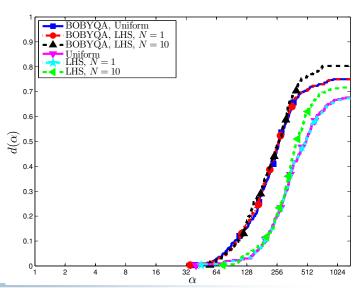
#### Problem setup:

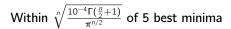
- ▶ 10 different GKLS problems
- ▶ 5 different seeds
- ▶ n = 2, ..., 7
- ► Same starting LHS sample of 10*n* points (except for uniform)
- ► Same (uniform)  $r_k$  value

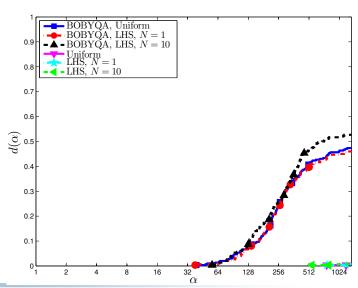


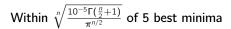


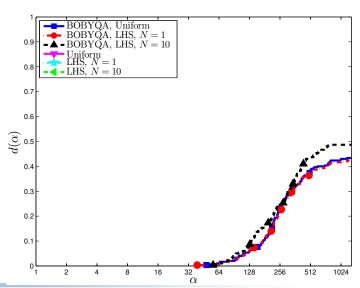


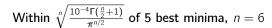


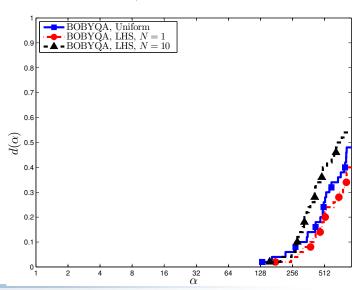


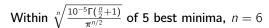


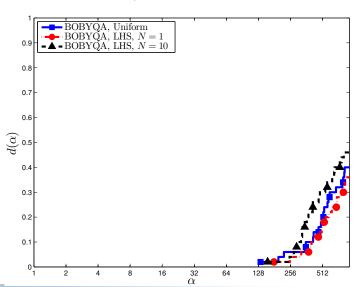


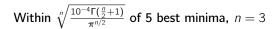


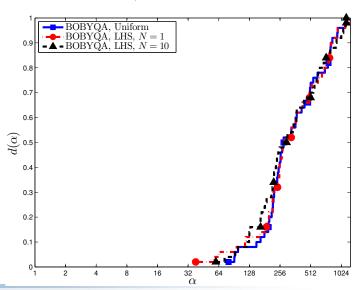


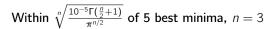


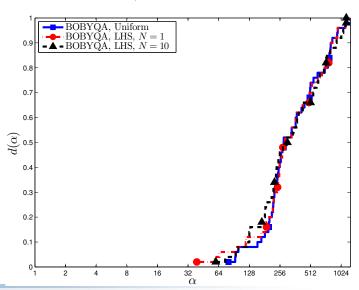




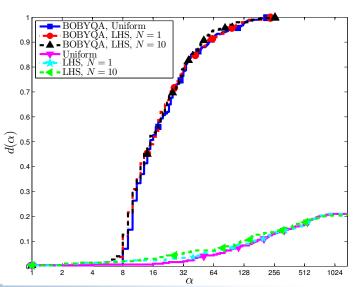




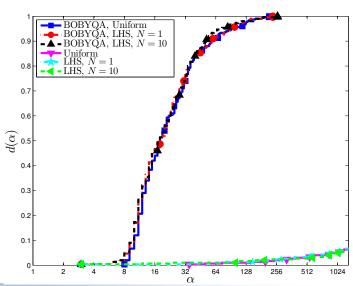




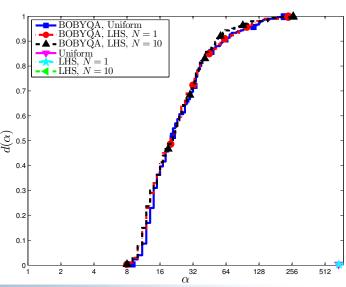
$$f(x) - f_{(1)}^* \le (1 - 10^{-2}) \left( f(x_0) - f_{(1)}^* \right)$$



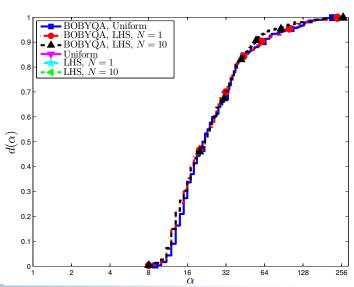
$$f(x) - f_{(1)}^* \le (1 - 10^{-3}) \left( f(x_0) - f_{(1)}^* \right)$$



$$f(x) - f_{(1)}^* \le (1 - 10^{-4}) \left( f(x_0) - f_{(1)}^* \right)$$



$$f(x) - f_{(1)}^* \le (1 - 10^{-5}) \left( f(x_0) - f_{(1)}^* \right)$$



#### **Closing Remarks**

► Concurrent function evaluations can locate multiple minima while efficiently finding a global minimum.

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- Concurrent function evaluations can locate multiple minima while efficiently finding a global minimum.
- ► Latin hypercube sampling appears to help find more minima in higher-dimensional problems.

#### Questions:

- ► Finding (or designing) the best local solver for our framework?
- Best way to process the queue?

#### **AAMLM**

#### Algorithm 3: AAMLM

```
Give each worker a point to evaluate for k = 1, 2, \dots do
```

Receive from (longest waiting) worker w that has evaluated f Update  $\mathcal{H}_k$  and  $r_k$ 

if point evaluated by  $\boldsymbol{w}$  is from an active run then

if Run is complete then

Update  $X_k^*$ , and mark points inactive

else

 $\perp$  Add the next point in its localopt run (not in  $\mathcal{H}_k$ ) to  $Q_L$ 

Start run(s) at all point(s) satisfying (S1)–(S4), (L1)–(L6)

Add the subsequent point (not in  $\mathcal{H}_k$ ) from each run to  $Q_L$ 

Merge runs in  $Q_L$  with candidate minima within  $2\nu$  of each other Give w a point at which to evaluate f, either from  $Q_L$  or  $\mathcal{R}$ 



